Topological Constraints on the Charge Distributions for the Thomson Problem

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Abstract

The method of Morse theory is used to analyze the distributions of unit charges interacting through a repulsive force and constrained to move on the surface of a sphere – the Thomson problem. We find that, due to topological reasons, the system may organize itself in the form of pentagonal structures. This gives a qualitative account for the interesting "pentagonal buttons" discovered in recent numerical work.

Dedicated to Rafael Sorkin on his 60th birthday

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I. INTRODUCTION

The Thomson problem consists in determining the minimum energy configurations for a given collection of N unit like-sign electric charges constrained to move on the surface of a two-sphere of radius R [1]. The Coulomb energy of such a system is

$$E_C \sim \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \ , \tag{I.1}$$

where $\vec{r}_i$ is the radial coordinate of the i^{th} charge on the sphere. The actual values of the electric charge and of the dielectric constant of the medium are inessential for the qualitative considerations we are going to make throughout the paper.

This is an old and largely unsolved problem that, in its generalized version – i.e. for more general repulsive potentials as well as for topological defects rather than unit electric charges – finds applications ranging from superconductivity to biology.

In recent years, triggered by the seminal paper of reference [2], there has been a lot of interesting theoretical, numerical and experimental work on the generalized Thomson problem [3]. In [2] the authors deal with disclination defects constrained to move on a sphere. They show how an *effective* defect model, rather than the analysis of the actual elementary charges interaction, proves to be extremely reliable to describe (by numerical means) the ground state configurations in terms of the ratio of the defect core energies to the Young modulus. This way they provide interesting empirical *solutions* to the Thomson problem, presenting patterns the defects form on the surface of the sphere at the various energy thresholds.

We would like to understand the patterns formed the way described in [2], i.e. *why* these charges (defects) arrange themselves on the surface of the sphere following precise symmetry prescriptions. We would expect the distribution to have the property that each charge has the same environment. If such an assumption is made the charges should be distributed in a way that represents a *tiling* of the surface of the sphere.

The general problem of tiling a genus g surface, say Σ_g, can be solved in a simple way. Suppose we want to tile Σ_g with regular p-sided polygons (p-gons) assembled in such a way that each vertex is shared by (is a common vertex for) 3 p-gons, and each edge is shared by (is a common edge for) 2 p-gons. If k_p is the number of p-gons used[1] to tile Σ_g, the resulting *polyhedron* P has $V_P = 1/3 \sum_k k_p p$ vertices, $E_P = 1/2 \sum_k k_p p$ edges, and $F_P = \sum_k k_p$ faces, giving for the Euler characteristic $\chi(\Sigma_g) = V_P - E_P + F_P$, the following expression

$$\sum_k k_p(6-p) = 6\chi(\Sigma_g) = 6(2-2g) \ . \tag{I.2}$$

Generalization to the case of vertices shared by not always three p-gons can be easily constructed.

For the sphere $g = 0$, and if only *hexagons* and *pentagons* are used, there can be an arbitrary number of hexagons, but there must be exactly 12 pentagons. This follows from Eq.(I.2)

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[1]There are, for instance, k_5 5-gons (pentagons), k_6 6-gons (hexagons), k_7 7-gons (heptagons), etc.

$$\sum_k k_p(6-p) = k_5\,(6-5) + k_6\,(6-6) = 12 \tag{I.3}$$

hence $k_5 = 12$ and k_6 is arbitrary. If one also uses *heptagons* for the tiling of the sphere, then one has the interesting result

$$k_5 - k_7 = 12\ . \tag{I.4}$$

Thus, one can start off by tiling the sphere with an arbitrary number of hexagons and exactly twelve pentagons. Then one can go on by adding an arbitrary number of *pairs* pentagon-heptagon, but not a pentagon or a heptagon separately. Let us notice *en passant* that other ways of tiling the sphere are, of course, possible. For instance, if only equilateral triangles (3-gons) are used, then from Eq.(I.2) follows

$$k_3\ 3 = 12 \quad \text{or} \quad k_3 = 4\ , \tag{I.5}$$

that is the *tetrahedron*.

We are particularly interested in the 5-gon–6-gon–7-gon tiling because the authors of [2] consider the pentagons and heptagons as disclination defects in a sea of hexagons. They construct an effective theory for E_C in (I.1) in terms of interactions between the defects, the background charge distribution of hexagons merely providing the value of the effective Young modulus. They prove that for a sphere of large radius, distorting the curvature by the introduction of defects is not excessively expensive in terms of bending energy. A 5-gon defect makes the local curvature negative, while a 7-gon makes it positive. For a large spherical system, therefore, the introduction of a 5-gon–7-gon pair is an energetically reasonable way of joining a group of 12 charges. A calculation had to be carried out to see if such a charge configuration was energetically favored as compared to 12 charges organized on two additional hexagons.

They find that when the total number N of charges on the sphere exceeds a certain critical value of $\mathcal{O}(500)$, the system prefers to have a collection of 5-gons and 7-gons arranged in the form of a linear chain of alternating 5-gon–7-gon sequence ("scar"). For even larger values of N, the preferred form is what they name "pentagonal buttons". These are configurations of two nested circles, with five 5-gons placed on the outer circle, five 7-gons on the inner circle, and finally a 5-gon in the common center. As N further increases, the defect system formes more intricate patterns. A C_3–symmetric configuration of defects is noted.

In this paper we would like to give qualitative topological arguments suggesting why these different defect configurations – such as pentagonal buttons or C_3 symmetric configurations, discovered by numerical minimization of E_C – can appear. We shall do so by recalling in Section II how the topological methods of Morse [4] apply to second order phase transitions in crystals (as pioneered by Michel, see e.g. [5]) paving the way to the application to the Thomson problem we shall deal with in Section III. Section IV is devoted our conclusions.

II. SYMMETRY BREAKING, MORSE THEORY AND SELECTION RULES

A crystal has a density function $\rho(\vec{x})$ invariant under one of the finite crystallographic groups, say G

$$\rho(g\vec{x}) = \rho(\vec{x}) \quad \text{with} \quad g \in G \,, \tag{II.1}$$

where $\rho(\vec{x})dV$ is the probability to find an atom of the crystal in the volume dV. Not all finite groups acting on 3 spatial dimensions, $\vec{x} = (x_1, x_2, x_3)$, are crystallographic groups, i.e. actual symmetries of crystals in nature. For instance: O_h, the *octahedral* group, the largest symmetry group of the cube, is a crystallographic group, while I, the *icosahedral* group, largely used in [2] for the effective theory of E_C, is not.

Crystals undergo second order phase transitions. The theory of such transitions has been established by Landau [6]. The density function ρ changes smoothly from one phase to the other, while the symmetry group G suddenly changes to a subgroup $H \subset G$. The density function can then be decomposed as

$$\rho(\vec{x}) + \delta\rho(\vec{x}) \tag{II.2}$$

where ρ is G-symmetric, while $\delta\rho$ is H-symmetric, and, at temperatures below the critical value $T < T_c$, $\delta\rho = 0$, while for $T > T_c$ is $\delta\rho \neq 0$. As the function changes continuously during the transition, $\delta\rho$ is small near T_c.

These transitions are (proto-)typical examples of spontaneous symmetry breaking: The thermodynamic potential $\Phi(\rho, T, P)$ is always G-invariant[2]. For $T < T_c$ the vacuum is G-invariant, realizing an explicitly symmetric phase; for $T > T_c$ the vacuum is H-invariant, realizing a spontaneously broken symmetric phase. By *vacuum* here we mean the ρ configuration that minimizes the functional $\Phi(\rho)$ for the given values of T and P.

Thus, given a G-symmetric crystal (ρ and Φ) one can select the sub-group H into which the crystal will make the transition, among the allowed subgroups of G, by finding the minimum of Φ with respect to ρ. Using physical reasonings Landau assumed that, near T_c, Φ is a polynomial in ρ of three terms of order zero, two and four (the Landau polynomial).

As ρ is a G-invariant function, it can be expanded in the basis of the functions $\{\phi_i(\vec{x})\}_{i=1,\dots,\mathrm{ord}(G)}$, where $\mathrm{ord}(G)$ is the number of elements (order) of the finite group G, and

$$\phi_i(\vec{x}) = \sum_{j=1}^{\mathrm{ord}(G)} D_{ij}[g]\phi_j(\vec{x}) \quad i = 1, ..., \mathrm{ord}(G) \,, \tag{II.3}$$

for any $g \in G$. The matrices $\{D_{ij}\}$ realize a reducible representation of G. Being ρ real, the representation is necessarily orthogonal.

In particular

$$\delta\rho(\vec{x}) = \sum_{i=1}^{\mathrm{ord}(G)} \eta_i \phi_i(\vec{x}) \tag{II.4}$$

and

$$\delta\rho'(\vec{x}) = \delta\rho(g\vec{x}) = \sum_{i=1}^{\mathrm{ord}(G)} {\eta'}_i \phi_i(\vec{x}) \tag{II.5}$$

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[2]This is so because it cannot depend on coordinates, hence, in particular, is invariant under G.

with ${\eta'}_i = \sum_j D_{ij}[g]\eta_j$. The η_is are the *order parameters* of the phase transition ($\eta_i = 0$ at $T < T_c$, $\eta_i \neq 0$ at $T > T_c$), hence the thermodynamic potential will be minimized with respect to these quantities $\Phi(\vec{\eta})$. The reducible set $\{\eta_i\}$ can be decomposed into irreducible sub-sets $\{\eta_i^a\}$ where

$$\eta_i^a = \sum_{b=1}^{n} d_{ab}[g]\eta_i^b \quad a = 1, ..., n \ , \tag{II.6}$$

the $d_{ab}[g]$s being the $n \times n$ irreducible matrix-blocks in the $\mathrm{ord}(G) \times \mathrm{ord}(G)$ matrices $D_{ij}[g]$ and, supposing there are m such irreducible representations of dimension $n_1, n_2, ..., n_m$, we have

$$n_1^2 + n_2^2 + ... + n_m^2 = \mathrm{ord}(G) \ . \tag{II.7}$$

Note that $\{\eta_i^a\}$ (or the corresponding $\{\phi_i^a\}$) is not a complete set. Nonetheless, it is only one such sets that is needed to expand $\delta\rho$ near T_c [6]. Thus, the problem of finding which way the G-symmetry of the crystal is spontaneously broken down to the smaller symmetry of one of its subgroups – say H – boils down to the minimization of the real function(al)

$$\Phi : \vec{\eta} \in S^n \to \Phi(\vec{\eta}) \in R \tag{II.8}$$

where n is one of the m values in (II.7), and we added to R^n the point at infinity that, for stability, has to be included as a maximum, so that $R^n + \{\infty\} = S^n$. In what follows we shall take $n = 3$.

One way of solving this problem is, of course, to explicitly know the coefficients of the Landau polynomial that depend upon the details of the model. Many things, though, can be said about the critical points (minima, maxima, saddle points) of a real function like Φ in (II.8), *without knowing its explicit expression*, but rather exploiting the constraints associated with the topology of S^n, as shown in the mathematical work of Morse [4] (for a physically intuitive introduction see, e.g., [7]; for extensive applications to phase transitions in crystals see, e.g., [5]).

In a nutshell, Morse proved that, when a function is like Φ, i.e. smooth, real and defined over a compact differentiable manifold (as said, we shall focus on the case of S^3), then the following constraints hold

$$c_0 \geq b_0 \tag{II.9}$$

$$c_1 - c_0 \geq b_1 - b_0 \tag{II.10}$$

$$c_2 - c_1 + c_0 \geq b_2 - b_1 + b_0 \tag{II.11}$$

$$c_3 - c_2 + c_1 - c_0 = b_3 - b_2 + b_1 - b_0 \tag{II.12}$$

where c_ℓ is the number of critical points of Φ with index[3] ℓ ($\ell = 0$ are the minima, $\ell = 3$ the maxima, $0 < \ell < 3$ the saddle points), and the b_ℓs are the Betti numbers of S^3. Recall that

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[3]In the neighborhood of $\vec{x}_0$, a result of Morse theory states that the function f has a local description of the form

$$b_0(S^3) = 1 = b_3(S^3) \ , \tag{II.13}$$

while the other Betti numbers of S^3 are all zero. This is a powerful result: without knowing the actual form of the function, the topology of the manifold tells us that for each ℓ there are at least b_ℓ critical points with index ℓ

$$c_\ell \geq b_\ell \ . \tag{II.14}$$

For the case in point we know that Φ has at least one minimum ($b_0 = 1$) and at least one maximum ($b_3 = 1$). Furthermore, denoting by $\vec{\eta}^{(\ell)} \in S^3$ the critical point of Φ with index ℓ, and by $H^{(\ell)}$ the subgroup of G that leaves it invariant,

$$\eta_a^{(\ell)} = \sum_{b=1}^{3} d_{ab}[h]\eta_b^{(\ell)} \quad h \in H^{(\ell)} \ , \tag{II.15}$$

the number of elements (order) of $H^{(\ell)}$ is simply related to c_ℓ

$$\mathrm{ord}(H^{(\ell)}) = \mathrm{ord}(G)/c_\ell \ . \tag{II.16}$$

It is a result of the theory of finite groups that $\mathrm{ord}(H^{(\ell)})$ as written in (II.16) is indeed an integer, the proof being based on the coset decomposition of G with respect to $H^{(\ell)}$ [8], [7].

The subgroup we are looking for is $H^{(0)}$, the symmetry of the vacuum configuration $\vec{\eta}^{(0)}$ and new symmetry H of the crystal beyond T_c. The constraints (II.9)-(II.12) and (II.16), the requirement to have *at least* two maxima (at $\vec{\eta}^{(3)} = \infty$ and at $\vec{\eta}^{(3)} = 0$), i.e. $c_3 \geq 2$, and the fact that the number of *real* solutions of $d\Phi/d\vec{\eta} = 0$ (with $\vec{\eta} \in S^3$ and Φ a fourth order polynomial) is bounded to be

$$c_0 + c_1 + c_2 + c_3 \leq 3^3 + 1 = 28 \ , \tag{II.17}$$

prove to be enough to identify the permitted $H^{(0)}$s! Which one is the actual H of the crystal after the spontaneous breaking of symmetry $G \hookrightarrow H$, of course, depends upon the particular physical situation under investigation.

Examples are crystalline structures, such as the alloy Cu-Zn, that exhibit the octahedral symmetry, whose group O_h has order 48. The subgroups of O_h allowed by the requirement to be crystallographic groups, have order 8, 6, 4 and 2. Carrying on the analysis outlined above furnishes: $\mathrm{ord}(H^{(0)}) = 6$, which corresponds to C_{3v}, and $\mathrm{ord}(H^{(0)}) = 8$, which corresponds to C_{4v} (recall that $\mathrm{ord}(C_n) = n$ and $\mathrm{ord}(C_{nv}) = 2n$). This means that C_{3v} and C_{4v} are *selected* as the only possible symmetries of a crystal, originally O_h-symmetric, undergoing a second order phase transition. More on this can be found in [5] and in [7].

$$f(\vec{x}) = f(\vec{x}_0) - y_1^2 - y_2^2 - \cdots - y_\ell^2 + y_{\ell+1}^2 + \cdots + y_{\dim M}^2 \ ,$$

where $y_i = (\vec{x} - \vec{x}_0)_i$ is the i^{th} coordinate of the vector $\vec{x} - \vec{x}_0$, and $\dim M$ is the dimension of the manifold M. The index ℓ of the critical point $\vec{x}_0$ refers to the number of negative terms present in the local description of $f(\vec{x})$. Then $\ell = 0$ means that no negative y^2 term is present in the local representation for f, so that the critical point is a local *minimum*. Similarly if $\ell = \dim M$, then it means that f decreases in value in all the $\dim M$ directions of the manifold, hence this critical point is a *maximum*.

III. THE THOMSON PROBLEM IN THE ICOSAHEDRAL APPROXIMATION

We shall now extensively rely on the model built up in [2], which deals with a system of topological defects on the surface of a spherical elastic material. Our considerations will be qualitative in nature, hence we shall skip many of the details of that analysis and will focus only on the topological and group-theoretical aspects of the problem. This way we shall provide an explanation of (some) of the empirical results of that work with the hope that our analysis could provide useful insight for that problem and, more generally, for the Thomson problem.

The authors of [2] deal with a sphere, originally tiled with an arbitrary number of hexagons and exactly twelve pentagons. The topology of the sphere requires that the defects, emerging as *disclinations* in the underlying structure of hexagons, must be: first the initial 12 pentagons, then the pairs pentagons-heptagons. On this we commented in the Introduction. For interactions among the defects that are strong compared to the interactions among the particles forming the material, as collectively described by the Young modulus, (what in [2] is identified as the "large core" energy regime), the twelve pentagons are the only defects in the system and are at the vertices of an *icosahedron*, because this configuration minimizes the energy[4] E_C. In the "small core" energy regimes new defects are energetically allowed as 12-plets of pentagon-heptagon pairs, and again they prefer to arrange themselves at the vertices of icosahedra. The patterns these additional defects describe on the surface of the sphere is our concern.

To try to understand that, we shall apply the analysis of the previous Section by considering the energy as a functional of the density function. Thus we shall regard E_C as a map

$$E_C : \vec{\eta} \in S^n \to R \,, \tag{III.1}$$

where, as explained, n is related to the symmetry group, the icosahedral group I in this case, the point at infinity is added for stability as a maximum, and the notation is the same as before. In the large core energy regime E_C and its minimum[5] (vacuum) are I-symmetric. In the small core energy regimes we shall make the approximation that E_C is still I-symmetric[6], but the vacua will only be invariant under a subgroup of I. This way we are dealing with the spontaneous breaking of the icosahedral symmetry into smaller symmetries we want to determine.

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[4]We shall still call the energy E_C. This is a clear abuse of notation because the energy here is quite more complicated than the expression given in (I.1). Nonetheless, for our considerations the actual form of the function is not important.

[5]Recall that (in the language of the Morse inequalities) $c_0 = \mathrm{ord}(I)/\mathrm{ord}(I) = 1$.

[6]That the I-symmetry of E_C in the small core energy regimes is a good approximation is a result we borrow from [2], where it is shown that indeed the energy is not severely modified by the introduction of these new defects.

The icosahedron is a polyhedron with twelve vertices, twenty faces and thirty edges. Its symmetry group I has 60 elements arranged into 5 conjugacy classes (the number of elements in the class is in parentheses) [8]: Identity (1), C_2 (15), C_3 (20), C_5 (12), C_5^2 (12). The subgroups of I are C_2, C_3, C_5 (of order 2, 3, 5, respectively) and those obtained by the coset decomposition of I with respect to them. The list of the *orders* of the subgroups is

$$\{2, 3, 5, 12, 20, 30\} \, . \tag{III.2}$$

Of course, by definition of polyhedron, the vertices of the icosahedron lie on the surface of a sphere. Nonetheless, we want to stress this here because, together with the topological constraints on the tiling and the choice of the irreducible representation of I relevant for the problem in point (i.e. the *three-dimensional* one), it makes clear the role of the two-sphere in configuration space. These comments are also in order because the topology of a *different* sphere, the $S^n = S^3$ in (III.1), will now play an important role.

Near the phase transition we suppose that E_C is a polynomial of order four, just as for the thermodynamic potential Φ of crystals. Hence the number of real solutions of $E'_C = 0$ is bounded from above

$$c_0 + c_1 + c_2 + c_3 \leq 3^3 + 1 = 28 \, , \tag{III.3}$$

where the point at infinity is also added.

We can now use the relevant Morse inequalities for the function in (III.1) with $n = 3$

$$c_0 \geq 1 \tag{III.4}$$

$$c_0 \leq 1 + c_1 \tag{III.5}$$

$$c_0 + c_2 \geq 1 + c_1 \tag{III.6}$$

$$c_0 + c_2 = c_1 + c_3 \, . \tag{III.7}$$

These, the request that $c_3 \geq 2$ and the constraint (III.3) are what we need to identify the order of the allowed subgroups H^0. We just have to insert the given order from the list (III.2) into

$$c_0 = 60/\mathrm{ord}(H^0) \, . \tag{III.8}$$

The resulting list of allowed subgroups consistent with the Morse inequalities and with the constraint (III.3) is

$$\{5, 12, 20, 30\} \, . \tag{III.9}$$

Let us analyze the case $\mathrm{ord}(H^0) = 12$. In this case the I-symmetry has been broken in such a way that there are 5 distinct minima ($c_0 = 5$) connected by a C_5 transformation (recall that 12 is the order of the coset of I with respect to C_5). Each minimum corresponds to a new icosahedron of defects, thus, according to this argument, there would be 5 new icosahedra. But, as shown, the new defects cannot appear unless they are in pairs of 5-gons–7-gons, thus, being 5 odd, we *must* have 10 new icosahedra: 5 icosahedra of pentagons next to 5 icosahedra of heptagons. These are the pentagonal buttons found in [2]. It would

be interesting to see how the residual symmetry of order twelve is related to the way these buttons arrange themselves on the sphere which, according to [2], is at certain vertices of the rhombic tricontahedron.

Similarly the case $\mathrm{ord}(H^0) = 20$ refers to 3 distinct minima for the new symmetry, connected by a C_3 transformation. By means of the same constraint to have 5-gons–7-gons pairs, we would expect to see 6 new icosahedra at the time, while the numerical results show 7 such clusters. This discrepancy could be due to the approximations we are introducing, either for the invariance of the energy or of the order of the polynomial near the phase transition.

We find also the cases: $\mathrm{ord}(H^0) = 30$, which refers to 2 distinct minima connected by a C_2 transformation, and the case $\mathrm{ord}(H^0) = 5$ which means $H = C_5$, in the notation of the previous Section.

IV. CONCLUSIONS

We applied the method of Morse theory and second order phase transition in crystals to the Thomson problem in the icosahedral approximation of reference [2]. We are able to describe the pentagonal buttons and the C_3 symmetry found there, although this last one only to an approximated extent. We also notice residual symmetries of orders not seen in that numerical work. This does not necessarily means that these new symmetries are to be found exactly in form given, because the analysis we made might require further care in order to be applied to other cases.

Our results are qualitative and preliminary. For instance, within this approach we are not able to address the important issue of the various energy thresholds involved with the phase transitions. Thus we cannot say *when* the transitions happen. Nonetheless, we can address the question *why* these transitions occur and in such a general fashion that it is suitable, in principle, for a wide range of applications. Hence, we believe, the results presented here are interesting especially in the view of stimulating the discussion for a deeper understanding of the Thomson problem in general.

We also notice that, having clarified the topological origin of the pentagonal buttons and C_3-symmetric configurations, it is reasonable to argue that these configurations share some features of *solitons*, in the sense that they cannot be undone by a continuous transformation.

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